Ethanone, 1-(1,3-dimethyl-1H-indol-2-yl)-

Other names: Ketone, 1,3-dimethylindol-2-yl methyl
2-Acetyl-1,3-dimethylindole
1,3-Dimethyl-2-acetylindole
Inchi: InChI=1S/C12H13NO/c1-8-10-6-4-5-7-11(10)13(3)12(8)9(2)14/h4-7H,1-3H3
InchiKey: KMVJHDBDTPGOGY-UHFFFAOYSA-N
Formula: C12H13NO
SMILES: CC(=O)c1c(C)c2ccccc2n1C
Mol. weight [g/mol]: 187.24
CAS: 16244-26-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.70		Crippen Method
logp	2.689		Crippen Method
mcvol	152.570	ml/mol	McGowan Method
rinpol	1811.00		NIST Webbook
rinpol	1852.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16244261&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices